



>>Entry Name: 6-Hydroxyhexanoic acid, 9CI

Synonym(s): 6-Hydroxycaproic acid

CAS Registry Number: 1191-25-9

HOCH₂(CH₂)₄COOH

Molecular Formula: C₆H₁₂O₃

Molecular Weight: 132.159

Accurate Mass: 132.078645

Percentage Composition: C 54.53%; H 9.15%; O 36.32%

Physical Description: Liq.

Other Data: Polymerises on heating to cryst. polymer, Mp 53-5°

>>Derivative: Me ester

Molecular Formula: C₇H₁₄O₃

Molecular Weight: 146.186

Accurate Mass: 146.094295

Percentage Composition: C 57.51%; H 9.65%; O 32.83%

Physical Description: Oil

>>Derivative: Et ester

CAS Registry Number: 5299-60-5

Molecular Formula: C₈H₁₆O₃

Molecular Weight: 160.213

Accurate Mass: 160.109945

Percentage Composition: C 59.98%; H 10.07%; O 29.96%

Boiling Point: Bp₁₅ 134°

Density: d₄²⁰ 0.978

Refractive Index: n_D²⁰ 1.4390

Aldrich: 37480-6

Rare Chemicals Library: S9772-2

>>Derivative: Nitrile

Synonym(s): 6-Hydroxyhexanenitrile. 5-Cyano-1-pentanol. Pentamethylene cyanohydrin

CAS Registry Number: 2453-48-7

Molecular Formula: C₆H₁₁NO

Molecular Weight: 113.159

Accurate Mass: 113.084064

Percentage Composition: C 63.69%; H 9.80%; N 12.38%; O 14.14%

Physical Description: Liq.

Boiling Point: Bp₃ 97-98°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1040C, (*nmr*)

Robinson, R. *et al.*, *J.C.S.*, 1937, 371, (*synth*)

Heilbron, I. *et al.*, *J.C.S.*, 1947, 1588, (*synth*)

Nohira, H. *et al.*, *Bull. Chem. Soc. Jpn.*, 1965, **38**, 897, (*nitrile*)

U.K. Pat., 1968, 1 129 292; *CA*, **70**, 11132r, (*synth*)

Ger. Pat., 1970, 2 013 524; *CA*, **74**, 12620t, (*synth*)

Srinivasan, K.G. *et al.*, *J.A.C.S.*, 1978, **100**, 2789, (*nitrile*)

Binns, F. *et al.*, *J.C.S. Perkin 1*, 1993, 899, (*synth, ir, pmr*)